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Self-consistent ab initio calculations for photoionization and electron-ion recombination using the R-matrix method

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Abstract. Most astrophysical plasmas entail a balance between ionization and recombination. We present new results from the powerful R-matrix method which yields in an ab initio manner: (I) self-consistent photoionization and recombination cross sections using identical wavefunction expansions, (II) unified e-ion recombination rates at all temperatures of interest, incorporating non-resonant and resonant processes, radiative and dielectronic recombination (RR and DR), and (III) level-specific recombination rates for many excited atomic levels. RR and DR processes can not be measured or observed independently. In contrast to the shortcomings of simple (but computationally easy) approximations that unphysically treat RR and DR separately with different methods, emphasizing marginal effects for selected ions over small energy ranges, the R-matrix method naturally and compeletely accounts for e-ion recombination for all atomic systems.

Photoionization and recombination cross sections are compared with state-of-the-art experiments on synchrotron radiation sources and ion storage rings. Overall agreement between theory and experiments is within 10-20 %. For photoionization the comparison includes not only the ground state but also the metastable states, with highly resolved resonance structures. The recent experiments therefore support the estimated accuracy of the vast amount of photoionization data computed under the Opacity Project (OP), the Iron Project (IP), and related works using the R-matrix method.

The inverse processes of bound-free transitions may proceed as,
i) Photoionization (PI) and Radiative Recombination (RR) :

$$X^{+Z} + h\nu \rightleftharpoons X^{+Z+1} + \epsilon$$

ii) Autoionization (AI) and Dielectronic recombination (DR):

$$e + X^{+Z} \rightarrow (X^{+Z-1})^{**} \rightarrow \begin{cases} e + X^{+Z} & \text{AI} \\ X^{+Z-1} + h\nu & \text{DR} \end{cases}$$

The doubly excited autoionizing states introduce resonances in the cross sections. RR and DR are observed together in nature although one may dominate the other, and quantum mechanical interference between the two may vary from low-Z to high Z elements, also depending on ion charge z. A new unified method has been developed (Nahar & Pradhan 1994, 1995; Zhang, Nahar & Pradhan

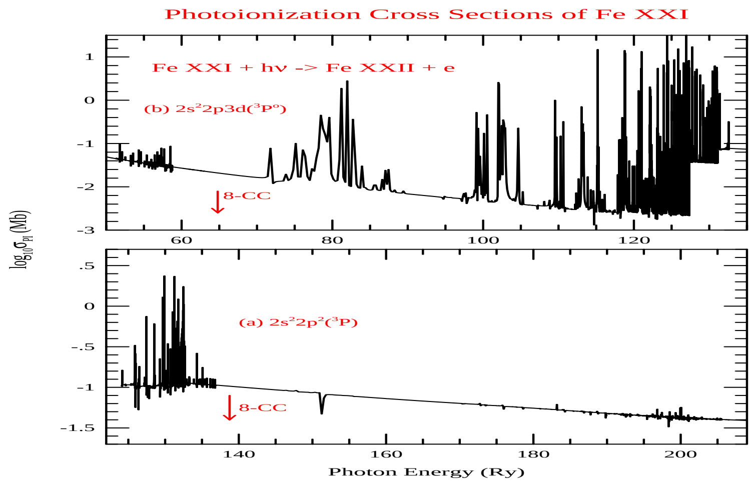

Figure 1. Photoionization cross sections, σ_{PI}, of ground $2s^2 2p^2(^3P)$ and excited $2s^2 2p3d(^3P^o)$ states of Fe XXI (Nahar 2002).

1999) that subsumes both RR and DR, and enables a self-consistent treatment for photoionization and (e + ion) recombination in astrophysical plasmas. Another review article in these proceedings discusses the throretical background of photoionization and total electron-ion recombination. We briefly note the points germaine to the self-consistent formulation using the R-matrix method in the close coupling approximation: (I) identical wavefunction expansion for the (e+ion) system is employed in ab initio calculations for photoionization and recombination, and (II) self-consistency *requires* an unified approach for (e+ion) recombination: $\alpha_R \to \alpha_{RR} + \alpha_{DR}$, as the natural inverse photoionization, (III) level-specific data is specifically obtained.

In contrast to the R-matrix formulation of the unified (e+ion) recombination, simpler methods treat RR and DR separately in the independent resonance approximation (e.g. Gorczyca et al. 2002). While this unphysical separation may not be too inaccurate for some highly charged ions, it must necessarily fail for all ions with strong coupling, such as the low ionization stages of iron Fe I - V (see the review article by the author). Simpler methods also tend to unduly emphasize issues of marginal general importance, such as radiation damping of a few high-n resonances, in the calculation of total recombination rates.

Fig. 1 presents photoionization cross sections, σ_{PI}, of the ground $2s^2 2p^2(^3P)$ and excited $2s^2 2p3d(^3P^o)$ states of Fe XXI (Nahar 2002, in preparation). The arrows show Rydberg autoionizing resonances arising from the 8 n=2 levels of the core ion (8CC wavefunction expansion). The ground state state shows significant resonances below the n=2 levels only. However, the large resonant features for the excited $^3P^o$ state are due to the n=3 thresholds, and enhance the effective cross section considerably at energies much higher than the n=2.

The R-matrix results may be compared to state-of-the-art experiments on synchrotron radiation sources for photoionization, and on heavy ion storage rings for recombination, which display heretofore unprecedented detail in resonances

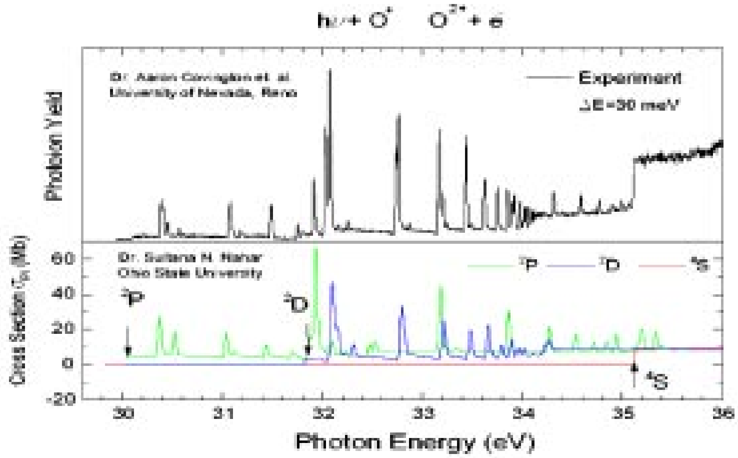

Figure 2. Comparison of theoretical and experimental photoionization cross sections of the metastable $2s^22p^3(^2P^o, ^2D^o)$ states of O II.

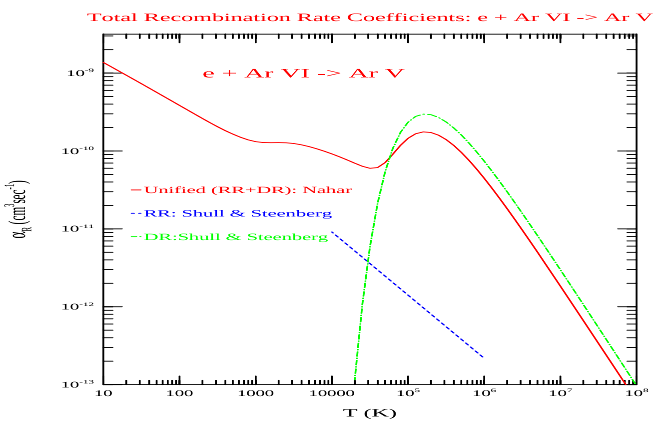

Figure 3. Total unified recombination rate coefficient of Ar V.

and background cross sections, and thereby calibrate the theoretical data precisely. An example of the comparison between the theory and experiment for σ_{PI} of ground and metastable states, $2s^22p^3(^4S^o, ^2D^o, ^2P^o)$, of O II is shown in Fig. 2 (Covington et al. 2001). Theoretical results (bottom panel) were obtained before the experiments were carried out, and helped to identify the resonances for the $^2P^o$ (green curve), and $^2D^o$ (blue curve) states respectively, in the total experimentally measured cross section (top panal).

The unified total electron-ion recombination rate coefficient, α_R, is obtained from the sum of photorecombination contributions to a large number of bound states, and to the rest of all highly excited states up to $n = \infty$ via DR. Fig. 3 presents α_R of e + Ar VI $\rightarrow$ Ar V (Nahar 2000). Total unified -red; RR - blue; DR (high-T) - green. Typically, the total α_R is high at low T (RR limit), and decreases before rising again due to dominance by DR. However, low-T "bumps" may exist due to autoionizing resonances in the low-energy region.

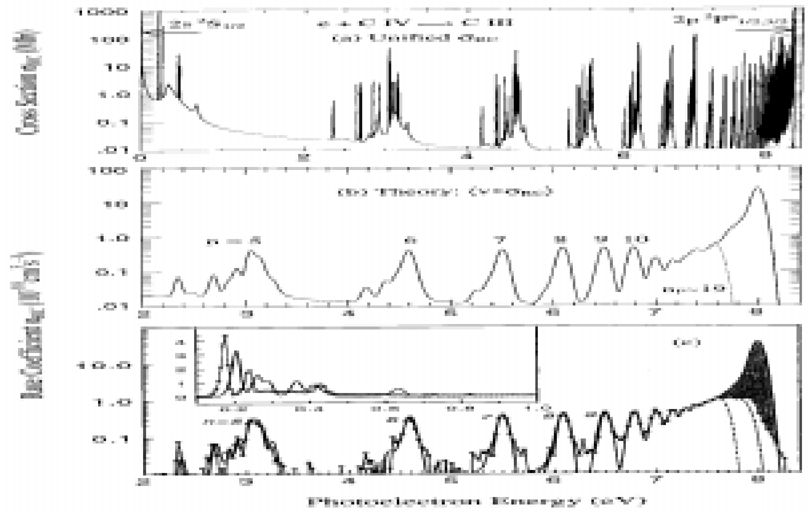

Figure 4. Comparison of theoretical and experimental recombination rate of C III (Pradhan et al. 2001).

The unified recombination cross sections (σ_{RC}) and rates have been benchmarded with experimental measurements, to about 10-15%. Fig. 4(a) shows the detailed unified σ_{RC} for (e + C IV) in the $1s^22s(^2S_{1/2} - -1s^22p(^2P^o_{1/2,3/2})$ region. The computed rate coefficient $v * \sigma_R$ is convolved with a gaussian experimental beamwidth (Fig. 4b), and compared with experimental results from the heavy-ion Test Storage Ring (Fig. 4c, Schippers et al. 2001). The present unified σ_{RC} in 4(a) show considerably more detail than the experimental results, but the convolved results agree to $\sim 15\%$ for individual n-complexes of resonances.

Self-consistent sets of atomic data for photoionization, recombination are obtained and should lead to more accurate astrophysical photoionization models.

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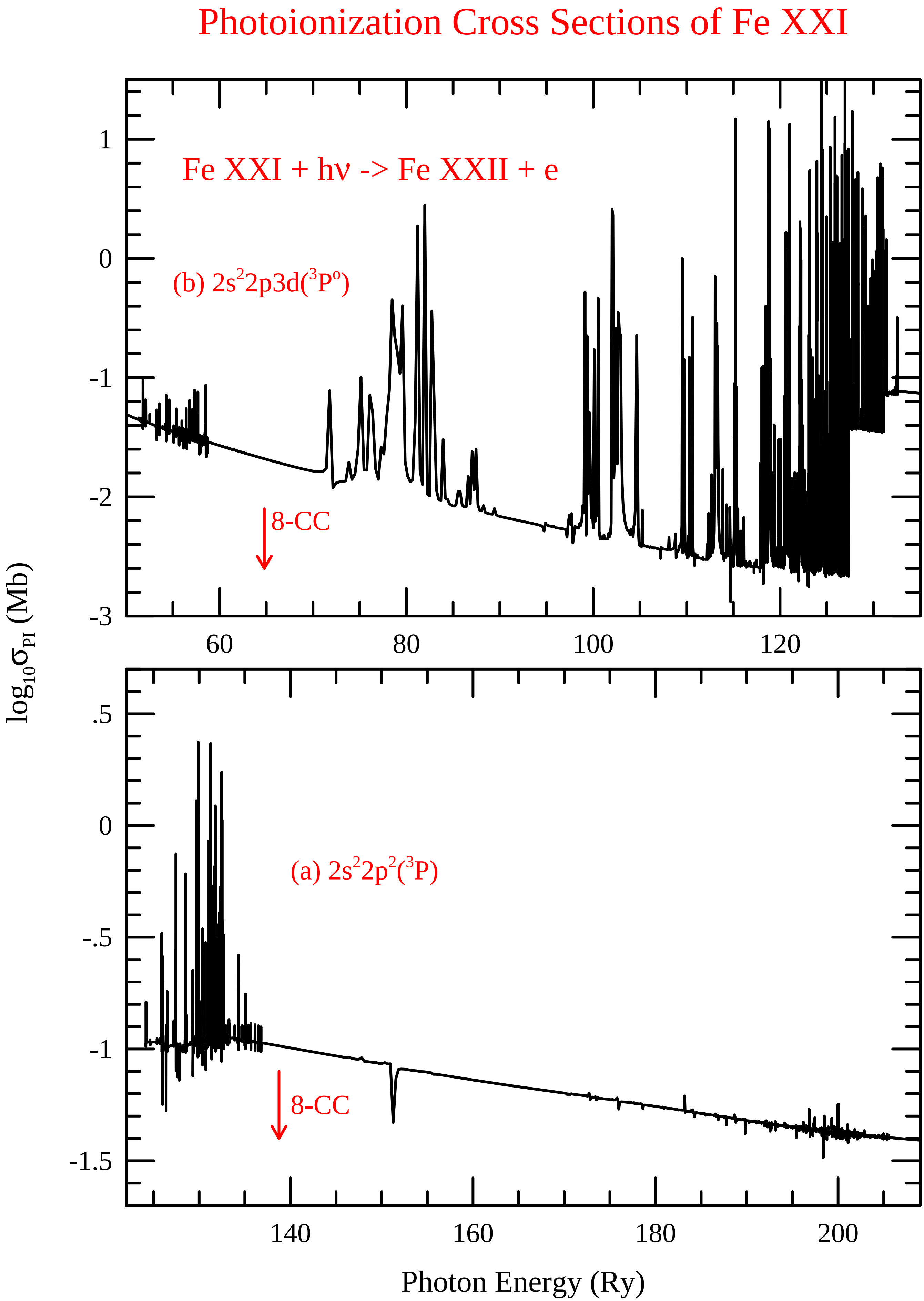

Photoionization Cross Sections of Fe XXI
Fe XXI + hν -> Fe XXII + e
(b) 2s22p3d(3Po)
8-CC
(a) 2s22p2(3P)
8-CC
log10σPI (Mb)
Photon Energy (Ry)
1
0
-1
-2
-3
60
80
100
120
.5
0
-.5
-1
-1.5
140
160
180
200

Total Recombination Rate Coefficients: e + Ar VI -> Ar V